Access DB# 93548

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Robert D. Harlan Examiner #: 77263 Date: 5/7/03
Art Unit: 1713 Phone Number 306-5926 Serial Number: 09/936,902
Mail Box and Bldg/Room Location: CP3-7A09 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.
****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

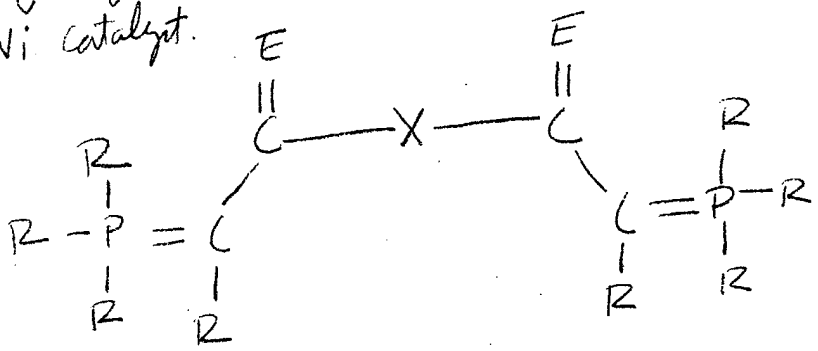
Title of Invention: Method for polymerizing olefin

Inventors (please provide full names): Tomov etal

Earliest Priority Filing Date: 09-19-01

***For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.**

Please search for the following ligand as part of a Ni catalyst.



R is alkyl or phenyl

X is  or $-CH_2-CH_2-$ or $-CH_2-$

E = O, S

(Not much for compounds with the metal. A few hits on the organic ligand alone.)

****

STAFF USE ONLY	Type of Search		Vendors and cost where applicable	
Searcher: Ed	NA Sequence (#)		STN	$205.89
Searcher Phone #:	AA Sequence (#)		Dialog	
Searcher Location:	Structure (#)	3	Questel/Orbit	
Date Searcher Picked Up:	Bibliographic		Dr.Link	
Date Completed: 5-8-03	Litigation		Lexis/Nexis	
Searcher Prep & Review Time: 5	Fulltext		Sequence Systems	
Clerical Prep Time:	Patent Family		WWW/Internet	
Online Time: 60	Other		Other (specify)	

PTO-1590 (1-2000)

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FILE 'REGISTRY' ENTERED AT 12:33:59 ON 09 MAY 2003
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     FILE 'REGISTRY' ENTERED AT 12:00:52 ON 09 MAY 2003
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L4                STR L1
L5              0 S L4 AND L2
L6                STR L2
L7              0 S L4 AND L6
L8                STR L4
L9              0 S L8 AND L6
L10             0 S L8 AND L6 FUL

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                  SAV L13 HAR902/A
L14             0 S L8 AND L6 SSS SAM SUB=L13
L15             0 S L8 AND L6 SSS FUL SUB=L13
L16            12 S L13 AND 1907-2001/PY

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L6                STR

M 1


NODE ATTRIBUTES:
NSPEC   IS RC     AT   1
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   1

STEREO ATTRIBUTES: NONE
L8                STR
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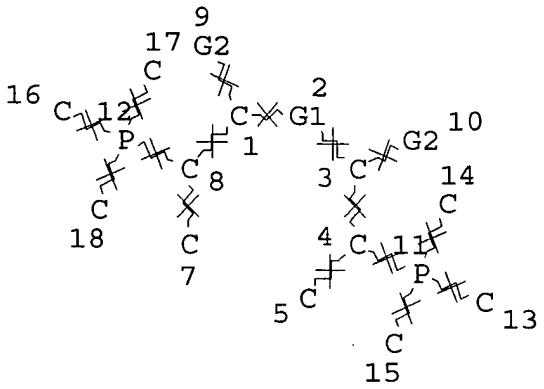

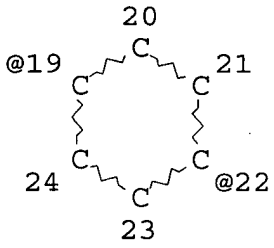

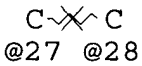

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VAR G2=O/S
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NSPEC IS RC AT 7
NSPEC IS RC AT 13
NSPEC IS RC AT 14
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NSPEC IS RC AT 18
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE
L10 0 SEA FILE=REGISTRY SSS FUL L8 AND L6

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SEARCH TIME: 00.00.01

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COPYRIGHT (c) 2003 Beilstein-Institut zur Foerderung der Chemischen Wissen
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FILE RELOADED ON OCTOBER 20, 2002
FILE LAST UPDATED ON APRIL 10, 2003

FILE COVERS 1771 TO 2003.


=> d l13 que stat
L8                STR
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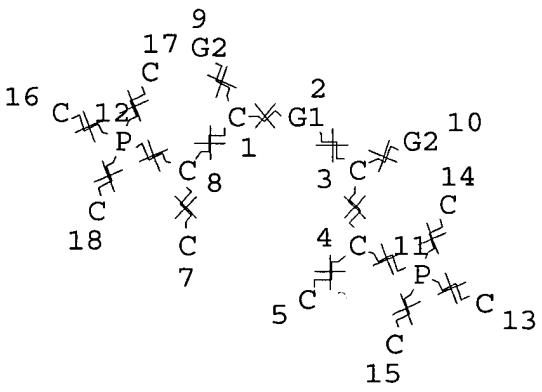

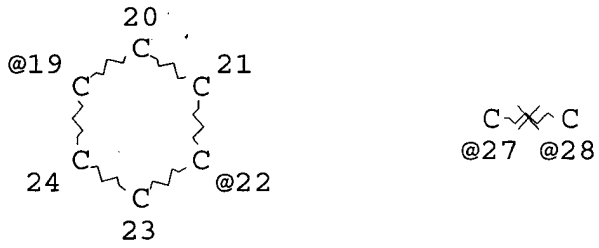


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VAR G1=19-1 22-3/27-1 28-3/C
VAR G2=O/S
NODE ATTRIBUTES:
NSPEC   IS RC     AT   5
NSPEC   IS RC     AT   7
NSPEC   IS RC     AT  13
NSPEC   IS RC     AT  14
NSPEC   IS RC     AT  15
NSPEC   IS RC     AT  16
NSPEC   IS RC     AT  17
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NSPEC IS RC AT 18
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 25

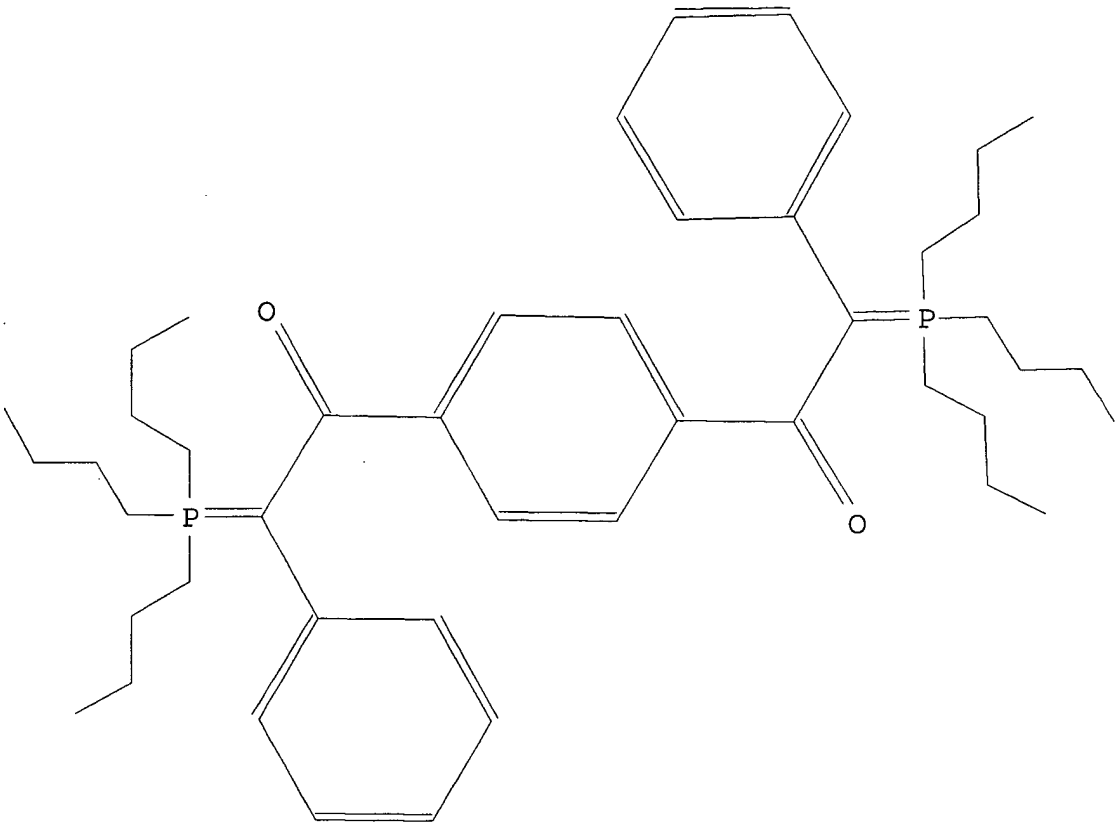
STEREO ATTRIBUTES: NONE
L13 13 SEA FILE=BEILSTEIN SSS FUL L8

100.0% PROCESSED 1131 ITERATIONS 13 ANSWERS
SEARCH TIME: 00.00.06

=> d l16 2,4,6,8 all

L16 ANSWER 2 OF 12 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN):	8379815
Chemical Name (CN):	1,4-bis<(phenyl)(tributylphosphoranylidene)acetyl>benzene
Autonom Name (AUN):	2-phenyl-1-<4-<phenyl-(tributyl-.lambda.5-phosphanylidene)-acetyl>-phenyl>-2-(tributyl-.lambda.5-phosphanylidene)-ethanone
Molec. Formula (MF):	C46 H68 O2 P2
Molecular Weight (MW):	714.99
Lawson Number (LN):	16730, 3764
Compound Type (CTYPE):	isocyclic
Constitution ID (CONSID):	7115632
Tautomer ID (TAUTID):	7904874
Entry Date (DED):	2000/03/08
Update Date (DUPD):	2000/03/08



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1
CPD	Crystal Property Description	1
IR	Infrared Spectrum	1
MP	Melting Point	1
NMR	Nuclear Magnetic Resonance	3

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Crystal Property Description:
CPD
(CPD): yellow
Reference(s):
1. Aitken, R. Alan; Drysdale, Martin J.; Hill, Lawrence; Lumbard, Keith W.; MacCallum, James R.; Seth, Shirley, Tetrahedron, CODEN: TETRAB, 55(36), <1999>, 11039 - 11050; BABS-6182053

Melting Point:

Value (MP) (Cel)	Ref.
177 - 180	1

Reference(s):
1. Aitken, R. Alan; Drysdale, Martin J.; Hill, Lawrence; Lumbard, Keith W.; MacCallum, James R.; Seth, Shirley, Tetrahedron, CODEN: TETRAB, 55(36), <1999>, 11039 - 11050; BABS-6182053

Nuclear Magnetic Resonance:
NMR
Coupling Nuclei (.NUI): 1H-1H
Solvents (.SOL): CDCl3
Frequency (.F): 300 MHz
Reference(s):
1. Aitken, R. Alan; Drysdale, Martin J.; Hill, Lawrence; Lumbard, Keith W.; MacCallum, James R.; Seth, Shirley, Tetrahedron, CODEN: TETRAB, 55(36), <1999>, 11039 - 11050; BABS-6182053

NMR
Description (.KW): Chemical shifts
Nucleus (.NUC): 1H
Solvents (.SOL): CDCl3
Frequency (.F): 300 MHz
Reference(s):
1. Aitken, R. Alan; Drysdale, Martin J.; Hill, Lawrence; Lumbard, Keith W.; MacCallum, James R.; Seth, Shirley, Tetrahedron, CODEN: TETRAB, 55(36), <1999>, 11039 - 11050; BABS-6182053

NMR
Description (.KW): Chemical shifts
Nucleus (.NUC): 31P
Solvents (.SOL): CDCl3
Frequency (.F): 32 MHz
Reference(s):

1. Aitken, R. Alan; Drysdale, Martin J.; Hill, Lawrence; Lumbard, Keith W.; MacCallum, James R.; Seth, Shirley, Tetrahedron, CODEN: TETRAB, 55(36), <1999>, 11039 - 11050; BABS-6182053

Infrared Spectrum:

Description (.KW)	Solvent (.SOL)	Ref.
Bands	nujol	1

Reference(s):
1. Aitken, R. Alan; Drysdale, Martin J.; Hill, Lawrence; Lumbard, Keith W.; MacCallum, James R.; Seth, Shirley, Tetrahedron, CODEN: TETRAB, 55(36), <1999>, 11039 - 11050; BABS-6182053

Reaction:
RX

Reaction ID (.ID):	5215853
Reactant BRN (.RBRN):	3776226, 607796
Reactant (.RCT):	benzyl-tributyl-phosphonium; chloride, terephthaloyl dichloride
Product BRN (.PBRN):	8379815
Product (.PRO):	2-phenyl-1-<4-<phenyl-(tributyl-.lambda.5-phosphanylidene)-acetyl>-phenyl>-2-(tributyl-.lambda.5-phosphanylidene)-ethanone
No. of React. Details (.NVAR):	1

Reaction Details:
RX

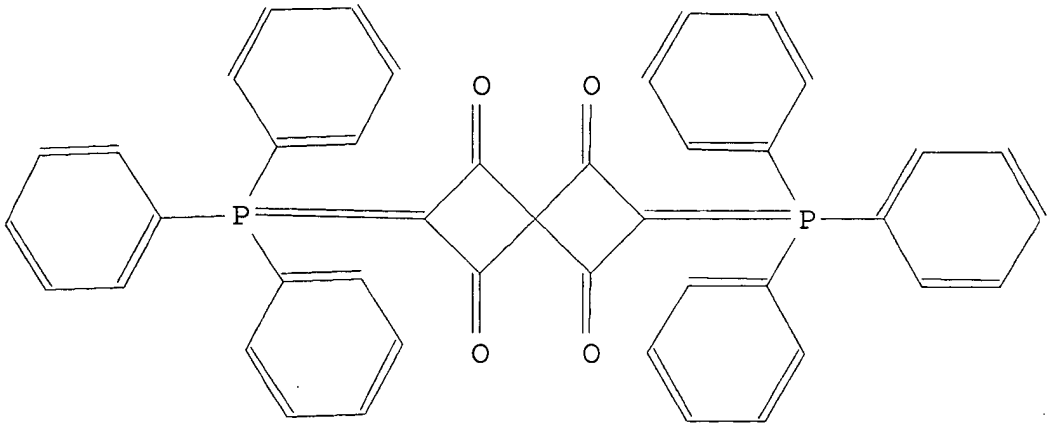
Reaction RID (.RID):	5215853.1
Reaction Classification (.CL):	Preparation
Yield (.YDT):	50 percent (BRN=8379815)
Reagent (.RGT):	BuLi
Solvent (.SOL):	tetrahydrofuran, hexane
Time (.TIM):	12 hour(s)
Reaction Type (.TYP):	Acylation, transylidation

Reference(s):
1. Aitken, R. Alan; Drysdale, Martin J.; Hill, Lawrence; Lumbard, Keith W.; MacCallum, James R.; Seth, Shirley, Tetrahedron, CODEN: TETRAB, 55(36), <1999>, 11039 - 11050; BABS-6182053

L16 ANSWER 4 OF 12 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN):	7453566
Chemical Name (CN):	2,6-bis-(triphenyl-.lambda.5-phosphanylidene)-spiro<3.3>heptane-

Autonom Name (AUN):	1,3,5,7-tetraone 2,6-bis-(triphenyl-.lambda.5-phosphanylidene)-spiro<3.3>heptane-1,3,5,7-tetraone
Molec. Formula (MF):	C43 H30 O4 P2
Molecular Weight (MW):	672.66
Lawson Number (LN):	16735, 16731
Compound Type (CTYPE):	isocyclic
Constitution ID (CONSID):	6392524
Tautomer ID (TAUTID):	7063132
Beilstein Citation (BSO):	6-16
Entry Date (DED):	1996/08/09
Update Date (DUPD):	1997/04/28



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
CDEN	Density (Crystal)	1
CRYPH	Crystal Phase	1

CSG	Crystal Space Group	1
CSYS	Crystal System	1
GEO	Interatomic Distanc and Angle	1
IR	Infrared Spectrum	1
MP	Melting Point	1
MS	Mass Spectrum	1
NMR	Nuclear Magnetic Resonance	4

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

Interatomic Distance and Angle:
GEO
Description (.KW): Interatomic distances and angles
Reference(s):
1. Pandolfo, Luciano; Facchin, Giacomo; Bertani, Roberta; Ganis, Paolo; Valle, Giovanni, Angew.Chem., CODEN: ANCEAD, 108(1), <1996>, 75-77; BABS-6009844

Melting Point:

Value (MP) (Cel)	Solvent (.SOL)	Ref.	Note
245 - 250	CH2Cl2	1	1

Reference(s):
1. Pandolfo, Luciano; Facchin, Giacomo; Bertani, Roberta; Ganis, Paolo; Valle, Giovanni, Angew.Chem., CODEN: ANCEAD, 108(1), <1996>, 75-77; BABS-6009844

Notes(s):
1. 50

Crystal Phase:
CRYPH
Description (.KW): Crystal structure determination
Note(s) (.COM): alpha=102.2 grad, beta=90.4 grad, .chi.=75.4 grad, a=14.99 Angstroem, b=18.95 Angstroem, c=12.91 Angstroem, n=2., Temperature: 298 K. Method of determination: Single Crystal X-ray Diffraction
Reference(s):

1. Pandolfo, Luciano; Facchin, Giacomo; Bertani, Roberta; Ganis, Paolo; Valle, Giovanni, Angew.Chem., CODEN: ANCEAD, 108(1), <1996>, 75-77; BABS-6009844

Crystal System:
CSYS

CSYS: triclinic
Reference(s):
1. Pandolfo, Luciano; Facchin, Giacomo; Bertani, Roberta; Ganis, Paolo; Valle, Giovanni, Angew.Chem., CODEN: ANCEAD, 108(1), <1996>, 75-77; BABS-6009844

Crystal Space Group:
CSG

CSG: C1i
Reference(s):
1. Pandolfo, Luciano; Facchin, Giacomo; Bertani, Roberta; Ganis, Paolo; Valle, Giovanni, Angew.Chem., CODEN: ANCEAD, 108(1), <1996>, 75-77; BABS-6009844

Crystal Density:

Value (CDEN) (g/cm**3)	Ref.
1.29	1

Reference(s):
1. Pandolfo, Luciano; Facchin, Giacomo; Bertani, Roberta; Ganis, Paolo; Valle, Giovanni, Angew.Chem., CODEN: ANCEAD, 108(1), <1996>, 75-77; BABS-6009844

Nuclear Magnetic Resonance:
NMR

Description (.KW): Chemical shifts
Nucleus (.NUC): 1H
Solvents (.SOL): CD2Cl2
Temperature (.T): 25 Cel
Reference(s):
1. Pandolfo, Luciano; Facchin, Giacomo; Bertani, Roberta; Ganis, Paolo; Valle, Giovanni, Angew.Chem., CODEN: ANCEAD, 108(1), <1996>, 75-77; BABS-6009844

NMR

Description (.KW): Chemical shifts
Nucleus (.NUC): 13C
Solvents (.SOL): CD2Cl2
Temperature (.T): 25 Cel
Reference(s):
1. Pandolfo, Luciano; Facchin, Giacomo; Bertani, Roberta; Ganis,

Paolo; Valle, Giovanni, Angew.Chem., CODEN: ANCEAD, 108(1), <1996>, 75-77; BABS-6009844

NMR

Description (.KW): Chemical shifts
Nucleus (.NUC): 31P
Solvents (.SOL): CD2Cl2
Temperature (.T): 25 Cel
Reference(s):
1. Pandolfo, Luciano; Facchin, Giacomo; Bertani, Roberta; Ganis, Paolo; Valle, Giovanni, Angew.Chem., CODEN: ANCEAD, 108(1), <1996>, 75-77; BABS-6009844

NMR

Description (.KW): Spin-spin coupling constants
Solvents (.SOL): CD2Cl2
Temperature (.T): 25 Cel
Note(s) (.COM): 31P-13C.
Reference(s):
1. Pandolfo, Luciano; Facchin, Giacomo; Bertani, Roberta; Ganis, Paolo; Valle, Giovanni, Angew.Chem., CODEN: ANCEAD, 108(1), <1996>, 75-77; BABS-6009844

Infrared Spectrum:

Description (.KW)	Solvent (.SOL)	Ref.	Note
Bands	nujol	1	1

Reference(s):
1. Pandolfo, Luciano; Facchin, Giacomo; Bertani, Roberta; Ganis, Paolo; Valle, Giovanni, Angew.Chem., CODEN: ANCEAD, 108(1), <1996>, 75-77; BABS-6009844

Notes(s):
1. 1662 cm**(-1)

Mass Spectrum:

MS

Description (.KW): spectrum
Note(s) (.COM): FAB (fast atom bombardment)
Reference(s):
1. Pandolfo, Luciano; Facchin, Giacomo; Bertani, Roberta; Ganis, Paolo; Valle, Giovanni, Angew.Chem., CODEN: ANCEAD, 108(1), <1996>, 75-77; BABS-6009844

Reaction:

RX

Reaction ID (.ID): 4420782
Reactant BRN (.RBRN): 1697986, 2811397

Reactant (.RCT): propadienedione, (triphenylphosphoranylidene)ethenone
Product BRN (.PBRN): 7453566
Product (.PRO): 2,6-bis-(triphenyl-.lambda.5-phosphanylidene)-spiro<3.3>heptane-1,3,5,7-tetraone
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 4420782.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 86 percent (BRN=7453566)
Solvent (.SOL): toluene
Other Conditions (.COND): Ambient temperature
Reference(s):
1. Pandolfo, Luciano; Facchin, Giacomo; Bertani, Roberta; Ganis, Paolo; Valle, Giovanni, Angew.Chem., CODEN: ANCEAD, 108(1), <1996>, 75-77; BABS-6009844

Reaction:
RX
Reaction ID (.ID): 4433110
Reactant BRN (.RBRN): 7453566, 505984
Reactant (.RCT): 2,6-bis-(triphenyl-.lambda.5-phosphanylidene)-spiro<3.3>heptane-1,3,5,7-tetraone, acetaldehyde
Product BRN (.PBRN): 7424608
Product (.PRO): 2,6-diethylidene-spiro<3.3>heptane-1,3,5,7-tetraone
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 4433110.1
Reaction Classification (.CL): Preparation
Solvent (.SOL): nitromethane
Temperature (.T): 60 Cel
Reference(s):
1. Pandolfo, Luciano; Facchin, Giacomo; Bertani, Roberta; Ganis, Paolo; Valle, Giovanni, Angew.Chem., CODEN: ANCEAD, 108(1), <1996>, 75-77; BABS-6009844

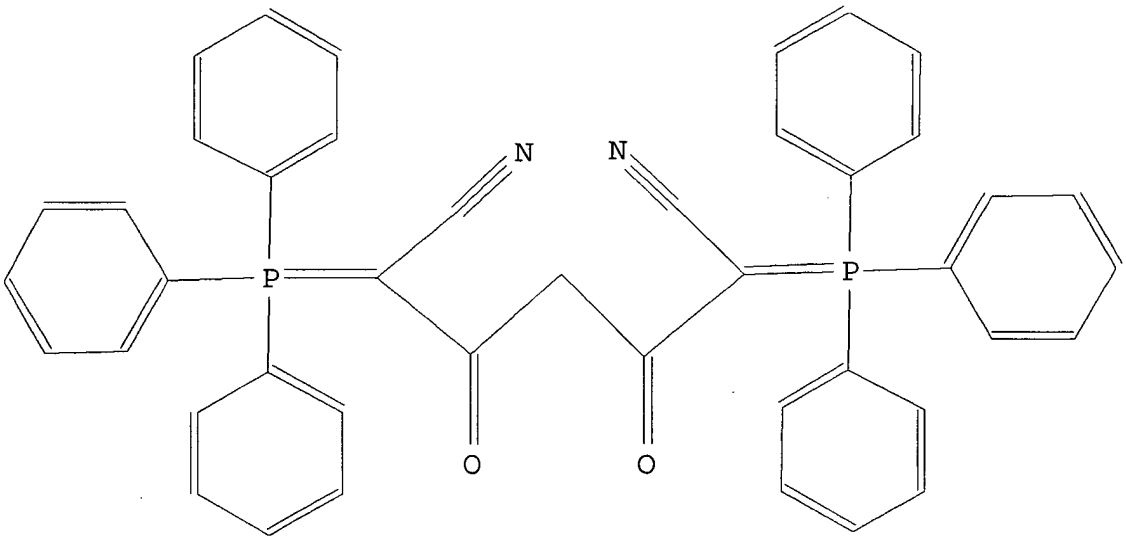
L16 ANSWER 6 OF 12 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN): 6840891
Fragm. Molec. Formula (FMF): C43 H32 N2 O2 P2 , C7 H8
Molecular Formula (MF): 2 C43 H32 N2 O2 P2 . 3 C7 H8
Molecular Weight (MW): 670.69, 92.14
Fragment BRN (FBRN): 6854445, 635760
Lawson Number (LN): 16731, 4108, 3763

Compound Type (CTYPE): isocyclic
Constitution ID (CONSID): 5945621
Tautomer ID (TAUTID): 6526783
Beilstein Citation (BSO): 6-16
Entry Date (DED): 1994/10/31
Update Date (DUPD): 1994/10/31

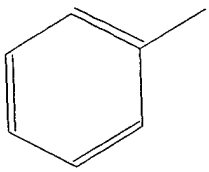
CM 1

FBRN 6854445
FMF C43 H32 N2 O2 P2



CM 2

FBRN 635760
FMF C7 H8



Field Availability:

Code	Name	Occurrence

BRN	Beilstein Records	1
FMF	Fragment Molecular Formula	2
MF	Molecular Formula	1
FW	Formular Weight	2
FBRN	Fragment BRN	2
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
CDEN	Density (Crystal)	1
CRYPH	Crystal Phase	1
CSG	Crystal Space Group	1
CSYS	Crystal System	1
GEO	Interatomic Distanc and Angle	1

Interatomic Distance and Angle:
GEO

Description (.KW): Interatomic distances and angles
Reference(s):
1. Pandolfo, Luciano; Facchin, Giacomo; Bertani, Roberta; Ganis, Paolo; Valle, Giovanni, Angew.Chem., CODEN: ANCEAD, 106(5), <1994>, 586-588; BABS-5894226

Crystal Phase:
CRYPH

Description (.KW): Crystal structure determination
Note(s) (.COM): alpha=77.8 grad, beta=86.5 grad, .chi.=62.6 grad, a=10.2 Angstroem, b=10.53 Angstroem, c=23.88 Angstroem, n=2., Temperature: 298 K. Method of determination: Single Crystal X-ray Diffraction
Reference(s):
1. Pandolfo, Luciano; Facchin, Giacomo; Bertani, Roberta; Ganis, Paolo; Valle, Giovanni, Angew.Chem., CODEN: ANCEAD, 106(5), <1994>, 586-588; BABS-5894226

Crystal System:
CSYS

CSYS: triclinic
Reference(s):
1. Pandolfo, Luciano; Facchin, Giacomo; Bertani, Roberta; Ganis, Paolo; Valle, Giovanni, Angew.Chem., CODEN: ANCEAD, 106(5), <1994>, 586-588; BABS-5894226

Crystal Space Group:
CSG

CSG: C1i

Reference(s):
1. Pandolfo, Luciano; Facchin, Giacomo; Bertani, Roberta; Ganis, Paolo; Valle, Giovanni, Angew.Chem., CODEN: ANCEAD, 106(5), <1994>, 586-588; BABS-5894226

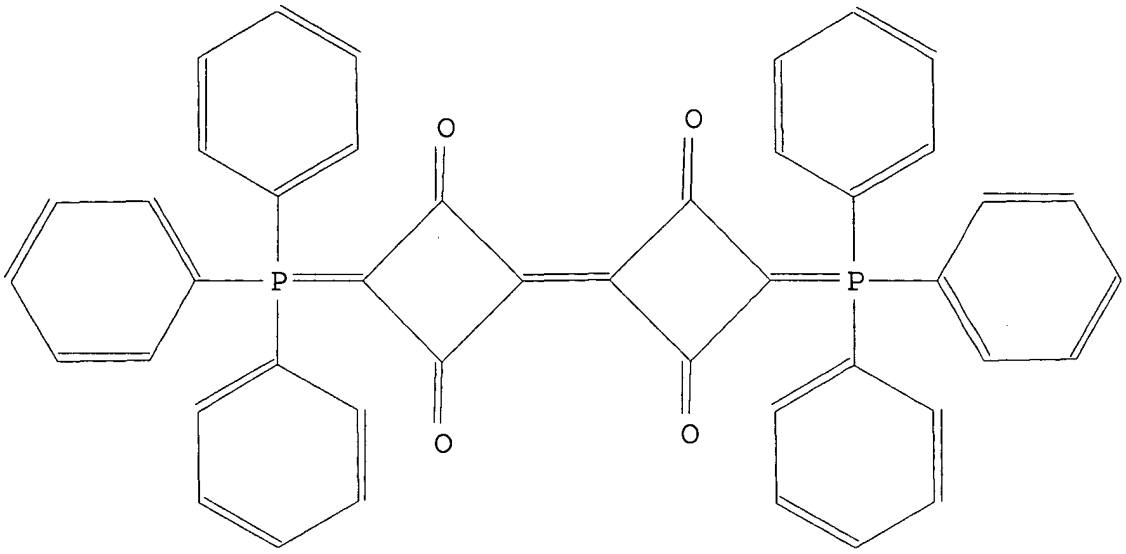
Crystal Density:

Value (CDEN) (g/cm**3)	Ref.
1.21	1

Reference(s):
1. Pandolfo, Luciano; Facchin, Giacomo; Bertani, Roberta; Ganis, Paolo; Valle, Giovanni, Angew.Chem., CODEN: ANCEAD, 106(5), <1994>, 586-588; BABS-5894226

L16 ANSWER 8 OF 12 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN):	6675719
Chemical Name (CN):	3,3'-bis-(triphenyl-.lambda.5-phosphanylidene)-bicyclobutylidene-2,4,2',4'-tetraone
Autonom Name (AUN):	3,3'-bis-(triphenyl-.lambda.5-phosphanylidene)-bicyclobutylidene-2,4,2',4'-tetraone
Molec. Formula (MF):	C44 H30 O4 P2
Molecular Weight (MW):	684.67
Lawson Number (LN):	16731, 16728
Compound Type (CTYPE):	isocyclic
Constitution ID (CONSID):	5787582
Tautomer ID (TAUTID):	6323323
Beilstein Citation (BSO):	6-16
Entry Date (DED):	1994/07/18
Update Date (DUPD):	1995/05/11



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
CDEN	Density (Crystal)	1
CRYPH	Crystal Phase	1
CSG	Crystal Space Group	1
CSYS	Crystal System	1
GEO	Interatomic Distanc and Angle	1
IR	Infrared Spectrum	1
MP	Melting Point	1
NMR	Nuclear Magnetic Resonance	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	3

RXREA Substance is Reaction Reactant 1
RXPRO Substance is Reaction Product 2

Interatomic Distance and Angle:
GEO
Description (.KW): Interatomic distances and angles
Reference(s):
1. Bestmann, Hans Juergen; Fuerst, Thomas G.; Schier, Annette, Angew.Chem., CODEN: ANCEAD, 105(12), <1993>, 1783-1784; BABS-5852222

Melting Point:

Value (MP) (Cel)	Ref.	Note
	1	1

Reference(s):
1. Bestmann, Hans Juergen; Fuerst, Thomas G.; Schier, Annette, Angew.Chem., CODEN: ANCEAD, 105(12), <1993>, 1783-1784; BABS-5852222

Notes(s):
1. Details: sintered at: 300 C - 360 C

Crystal Phase:
CRYPH
Description (.KW): Crystal structure determination
Note(s) (.COM): alpha=81.6 grad, beta=86.9 grad, .chi.=88 grad, a=9.28 Angstroem, b=9.31 Angstroem, c=9.95 Angstroem, n=1., Temperature: 22 C. Method of determination: X-ray Diffraction
Reference(s):
1. Bestmann, Hans Juergen; Fuerst, Thomas G.; Schier, Annette, Angew.Chem., CODEN: ANCEAD, 105(12), <1993>, 1783-1784; BABS-5852222

Crystal System:
CSYS
CSYS: triclinic
Reference(s):
1. Bestmann, Hans Juergen; Fuerst, Thomas G.; Schier, Annette, Angew.Chem., CODEN: ANCEAD, 105(12), <1993>, 1783-1784; BABS-5852222

Crystal Space Group:
CSG
CSG: C1i

Reference(s):
1. Bestmann, Hans Juergen; Fuerst, Thomas G.; Schier, Annette, Angew.Chem., CODEN: ANCEAD, 105(12), <1993>, 1783-1784; BABS-5852222

Crystal Density:

Value (CDEN) (g/cm**3)	Ref.
1.338	1

Reference(s):
1. Bestmann, Hans Juergen; Fuerst, Thomas G.; Schier, Annette, Angew.Chem., CODEN: ANCEAD, 105(12), <1993>, 1783-1784; BABS-5852222

Nuclear Magnetic Resonance:
NMR

Description (.KW):	Chemical shifts
Nucleus (.NUC):	31P
Solvents (.SOL):	CDCl3
Temperature (.T):	25 Cel

Reference(s):
1. Bestmann, Hans Juergen; Fuerst, Thomas G.; Schier, Annette, Angew.Chem., CODEN: ANCEAD, 105(12), <1993>, 1783-1784; BABS-5852222

Infrared Spectrum:

Description (.KW)	Solvent (.SOL)	Ref.	Note
Bands	KBr	1	1

Reference(s):
1. Bestmann, Hans Juergen; Fuerst, Thomas G.; Schier, Annette, Angew.Chem., CODEN: ANCEAD, 105(12), <1993>, 1783-1784; BABS-5852222

Notes(s):
1. 1650 - 1640 cm**(-1)

Reaction:
RX

Reaction ID (.ID):	2171987
Reactant BRN (.RBRN):	2795610
Reactant (.RCT):	2,4-bis-(triphenyl-.lambda.5-

phosphanylidene)-cyclobutane-1,3-dione
Product BRN (.PBRN): 6675719
Product (.PRO): 3,3'-bis-(triphenyl-.lambda.5-phosphanylidene)-bicyclobutylidene-2,4,2',4'-tetraone
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 2171987.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 98 percent (BRN=6675719)
Reagent (.RGT): N-p-tolylsulfonyl(phenyl)oxaziridine
Solvent (.SOL): diethyl ether
Reference(s):
1. Bestmann, Hans Juergen; Fuerst, Thomas G.; Schier, Annette, Angew.Chem., CODEN: ANCEAD, 105(12), <1993>, 1783-1784; BABS-5852222

Reaction:
RX
Reaction ID (.ID): 2171985
Reactant BRN (.RBRN): 2795610, 6657405
Reactant (.RCT): 2,4-bis-(triphenyl-.lambda.5-phosphanylidene)-cyclobutane-1,3-dione, 4-(triphenyl-.lambda.5-phosphanylidene)-cyclobutane-1,2,3-trione
Product BRN (.PBRN): 6675719
Product (.PRO): 3,3'-bis-(triphenyl-.lambda.5-phosphanylidene)-bicyclobutylidene-2,4,2',4'-tetraone
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 2171985.1
Reaction Classification (.CL): Preparation
Reference(s):
1. Bestmann, Hans Juergen; Fuerst, Thomas G.; Schier, Annette, Angew.Chem., CODEN: ANCEAD, 105(12), <1993>, 1783-1784; BABS-5852222

Reaction:
RX
Reaction ID (.ID): 3312996
Reactant BRN (.RBRN): 6675719, 605285
Reactant (.RCT): 3,3'-bis-(triphenyl-.lambda.5-phosphanylidene)-bicyclobutylidene-2,4,2',4'-tetraone, 2,3-dimethyl-buta-1,3-diene

Product BRN (.PBRN): 6678270
Product (.PRO): 10,11-dimethyl-2,7-bis-(triphenyl-.lambda.5-phosphanylidene)-dispiro<3.0.3.4>dodec-10-ene-1,3,6,8-tetraone
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 3312996.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 58 percent (BRN=6678270)
Solvent (.SOL): nitrobenzene
Time (.TIM): 24 hour(s)
Other Conditions (.COND): Heating
Reference(s):
1. Bestmann, Hans Juergen; Fuerst, Thomas G.; Schier, Annette, Angew.Chem., CODEN: ANCEAD, 105(12), <1993>, 1783-1784; BABS-5852222

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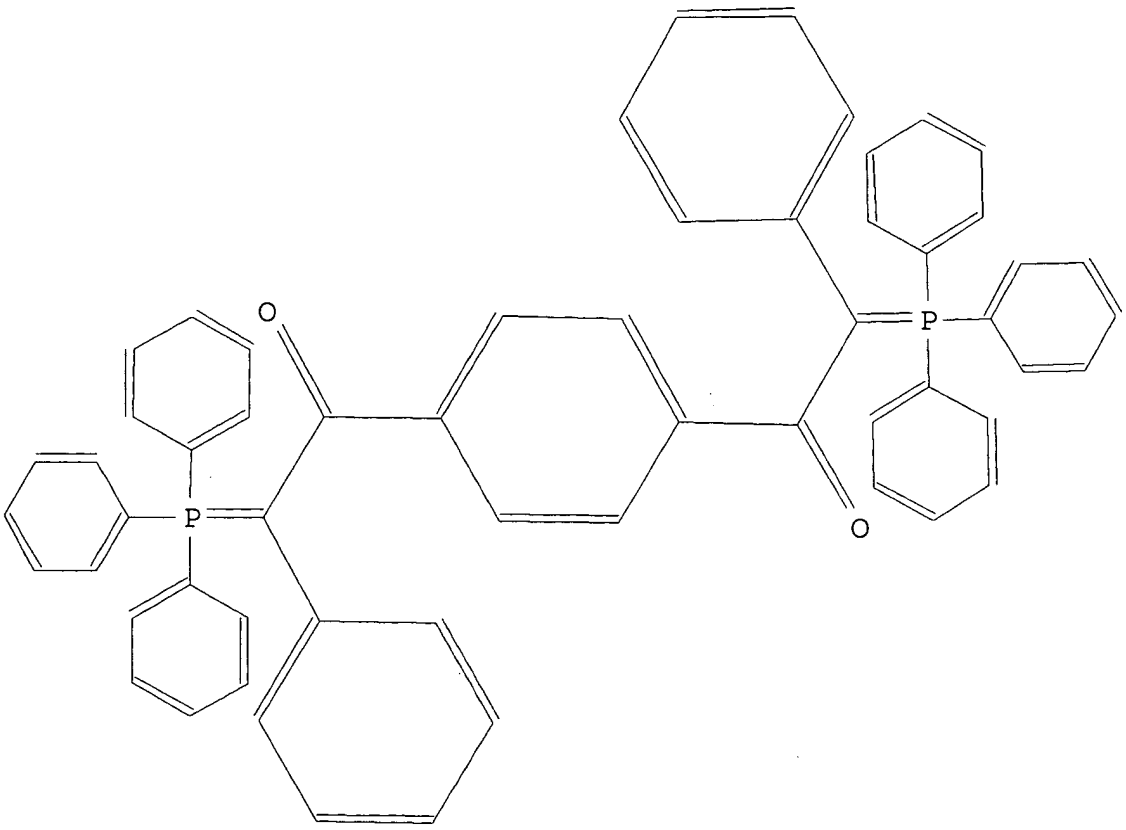
L16 ANSWER 3 OF 12 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN): 8379169
Chemical Name (CN): 1,4-bis<(phenyl)(triphenylphosphoranylidene)acetyl>benzene
Autonom Name (AUN): 2-phenyl-1-<4-<phenyl-(triphenyl-.lambda.5-phosphanylidene)-acetyl>-phenyl>-2-(triphenyl-.lambda.5-phosphanylidene)-ethanone
Molec. Formula (MF): C58 H44 O2 P2
Molecular Weight (MW): 834.93
Lawson Number (LN): 16731, 16730
Compound Type (CTYPE): isocyclic
Constitution ID (CONSID): 7115121
Tautomer ID (TAUTID): 7889594
Entry Date (DED): 2000/03/08
Update Date (DUPD): 2000/03/08



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1
CPD	Crystal Property Description	1
IR	Infrared Spectrum	1
MP	Melting Point	1
MS	Mass Spectrum	1
NMR	Nuclear Magnetic Resonance	4

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Crystal Property Description:
CPD
(CPD): yellow
Reference(s):
1. Aitken, R. Alan; Drysdale, Martin J.; Hill, Lawrence; Lumbard, Keith W.; MacCallum, James R.; Seth, Shirley, Tetrahedron, CODEN: TETRAB, 55(36), <1999>, 11039 - 11050; BABS-6182053

Melting Point:

Value (MP) (Cel)	Ref.
270 - 274	1

Reference(s):
1. Aitken, R. Alan; Drysdale, Martin J.; Hill, Lawrence; Lumbard, Keith W.; MacCallum, James R.; Seth, Shirley, Tetrahedron, CODEN: TETRAB, 55(36), <1999>, 11039 - 11050; BABS-6182053

Nuclear Magnetic Resonance:
NMR
Coupling Nuclei (.NUI): 31P-13C
Solvents (.SOL): CDCl3
Frequency (.F): 75 MHz
Reference(s):
1. Aitken, R. Alan; Drysdale, Martin J.; Hill, Lawrence; Lumbard, Keith W.; MacCallum, James R.; Seth, Shirley, Tetrahedron, CODEN: TETRAB, 55(36), <1999>, 11039 - 11050; BABS-6182053
NMR
Description (.KW): Chemical shifts
Nucleus (.NUC): 31P
Solvents (.SOL): CDCl3
Frequency (.F): 32 MHz
Reference(s):
1. Aitken, R. Alan; Drysdale, Martin J.; Hill, Lawrence; Lumbard, Keith W.; MacCallum, James R.; Seth, Shirley, Tetrahedron, CODEN: TETRAB, 55(36), <1999>, 11039 - 11050; BABS-6182053
NMR
Description (.KW): Chemical shifts
Nucleus (.NUC): 1H
Solvents (.SOL): CDCl3

Frequency (.F): 300 MHz
Reference(s):
1. Aitken, R. Alan; Drysdale, Martin J.; Hill, Lawrence; Lumbard, Keith W.; MacCallum, James R.; Seth, Shirley, Tetrahedron, CODEN: TETRAB, 55(36), <1999>, 11039 - 11050; BABS-6182053

NMR
Description (.KW): Chemical shifts
Nucleus (.NUC): 13C
Solvents (.SOL): CDCl3
Frequency (.F): 75 MHz
Reference(s):
1. Aitken, R. Alan; Drysdale, Martin J.; Hill, Lawrence; Lumbard, Keith W.; MacCallum, James R.; Seth, Shirley, Tetrahedron, CODEN: TETRAB, 55(36), <1999>, 11039 - 11050; BABS-6182053

Infrared Spectrum:

Description (.KW)	Solvent (.SOL)	Ref.
Bands	nujol	1

Reference(s):
1. Aitken, R. Alan; Drysdale, Martin J.; Hill, Lawrence; Lumbard, Keith W.; MacCallum, James R.; Seth, Shirley, Tetrahedron, CODEN: TETRAB, 55(36), <1999>, 11039 - 11050; BABS-6182053

Mass Spectrum:
MS
Description (.KW): spectrum, electron impact (EI)
Reference(s):
1. Aitken, R. Alan; Drysdale, Martin J.; Hill, Lawrence; Lumbard, Keith W.; MacCallum, James R.; Seth, Shirley, Tetrahedron, CODEN: TETRAB, 55(36), <1999>, 11039 - 11050; BABS-6182053

Reaction:
RX
Reaction ID (.ID): 5215852
Reactant BRN (.RBRN): 3599868, 607796
Reactant (.RCT): benzyl-triphenyl-phosphonium; chloride, terephthaloyl dichloride
Product BRN (.PBRN): 8379169
Product (.PRO): 2-phenyl-1-<4-<phenyl-(triphenyl-.lambda.5-phosphanylidene)-acetyl>-phenyl>-2-(triphenyl-.lambda.5-phosphanylidene)-ethanone
No. of React. Details (.NVAR): 1

Reaction Details:

RX

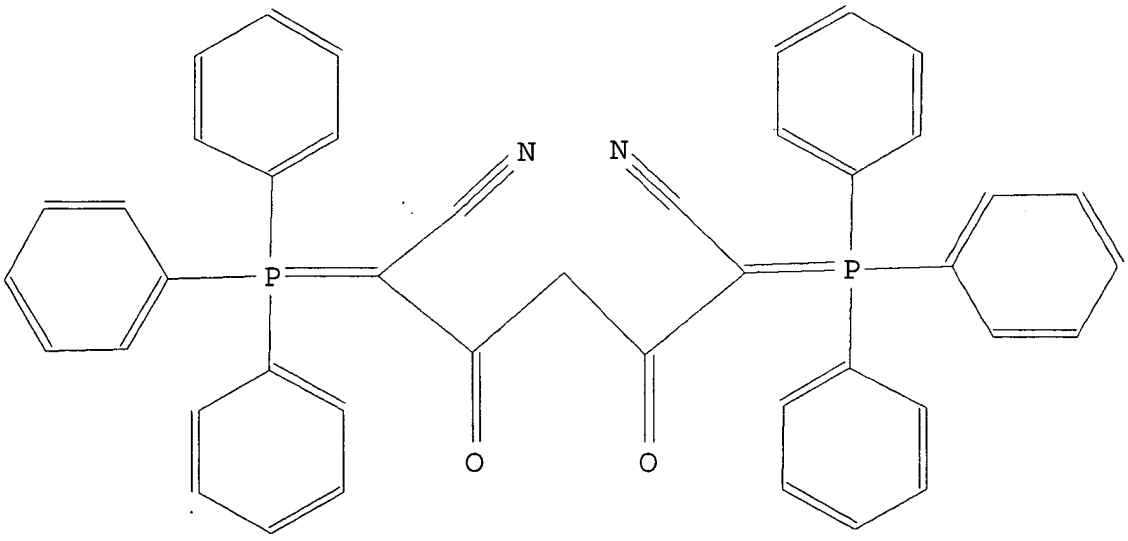
Reaction RID (.RID):	5215852.1
Reaction Classification (.CL):	Preparation
Yield (.YDT):	60 percent (BRN=8379169)
Reagent (.RGT):	BuLi
Solvent (.SOL):	tetrahydrofuran, hexane
Time (.TIM):	12 hour(s)
Reaction Type (.TYP):	Acylation, transylidation

Reference(s):

1. Aitken, R. Alan; Drysdale, Martin J.; Hill, Lawrence; Lumbard, Keith W.; MacCallum, James R.; Seth, Shirley, Tetrahedron, CODEN: TETRAB, 55(36), <1999>, 11039 - 11050; BABS-6182053

L16 ANSWER 5 OF 12 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN):	6854445
Chemical Name (CN):	1,3-bis(cyanomethylenetriphenylphosphorane)propane-1,3-dione
Autonom Name (AUN):	3,5-dioxo-2,6-bis-(triphenyl-.lambda.5-phosphanylidene)-heptanedinitrile
Molec. Formula (MF):	C43 H32 N2 O2 P2
Molecular Weight (MW):	670.69
Lawson Number (LN):	16731, 3763
Compound Type (CTYPE):	isocyclic
Constitution ID (CONSID):	5939736
Tautomer ID (TAUTID):	6516581
Beilstein Citation (BSO):	6-16
Entry Date (DED):	1994/10/31
Update Date (DUPD):	1996/04/26



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
IR	Infrared Spectrum	1
MP	Melting Point	1
MS	Mass Spectrum	2
NMR	Nuclear Magnetic Resonance	4

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Melting Point:

Value (MP) (Cel)	Ref.	Note
243 - 244	1	1

Reference(s):

1. Pandolfo, Luciano; Facchin, Giacomo; Bertani, Roberta; Ganis, Paolo; Valle, Giovanni, Angew.Chem., CODEN: ANCEAD, 106(5), <1994>, 586-588; BABS-5894226

Notes(s):

1. 50

Nuclear Magnetic Resonance:

NMR

Description (.KW): Chemical shifts

Nucleus (.NUC): 1H
Solvents (.SOL): CD2Cl2
Temperature (.T): 25 Cel
Reference(s):
1. Pandolfo, Luciano; Facchin, Giacomo; Bertani, Roberta; Ganis, Paolo; Valle, Giovanni, Angew.Chem., CODEN: ANCEAD, 106(5), <1994>, 586-588; BABS-5894226

NMR
Description (.KW): Chemical shifts
Nucleus (.NUC): 13C
Solvents (.SOL): CD2Cl2
Temperature (.T): 25 Cel
Reference(s):
1. Pandolfo, Luciano; Facchin, Giacomo; Bertani, Roberta; Ganis, Paolo; Valle, Giovanni, Angew.Chem., CODEN: ANCEAD, 106(5), <1994>, 586-588; BABS-5894226

NMR
Description (.KW): Chemical shifts
Nucleus (.NUC): 31P
Solvents (.SOL): CDCl3
Temperature (.T): 25 Cel
Reference(s):
1. Pandolfo, Luciano; Facchin, Giacomo; Bertani, Roberta; Ganis, Paolo; Valle, Giovanni, Angew.Chem., CODEN: ANCEAD, 106(5), <1994>, 586-588; BABS-5894226

NMR
Description (.KW): Spin-spin coupling constants
Solvents (.SOL): CD2Cl2
Temperature (.T): 25 Cel
Note(s) (.COM): 1H-13C, 31P-13C.
Reference(s):
1. Pandolfo, Luciano; Facchin, Giacomo; Bertani, Roberta; Ganis, Paolo; Valle, Giovanni, Angew.Chem., CODEN: ANCEAD, 106(5), <1994>, 586-588; BABS-5894226

Infrared Spectrum:

Description (.KW)	Solvent (.SOL)	Ref.	Note
Bands	nujol	1	1

Reference(s):
1. Pandolfo, Luciano; Facchin, Giacomo; Bertani, Roberta; Ganis, Paolo; Valle, Giovanni, Angew.Chem., CODEN: ANCEAD, 106(5), <1994>, 586-588; BABS-5894226

Notes(s):
1. 2175 - 1565 cm**(-1)

Mass Spectrum:
MS
Description (.KW): spectrum
Note(s) (.COM): FAB (fast atom bombardment)
Reference(s):
1. Pandolfo, Luciano; Facchin, Giacomo; Bertani, Roberta; Ganis, Paolo; Valle, Giovanni, Angew.Chem., CODEN: ANCEAD, 106(5), <1994>, 586-588; BABS-5894226

MS
Description (.KW): fragmentation pattern
Note(s) (.COM): FAB (fast atom bombardment), metastable ions
Reference(s):
1. Seraglia, Roberta; Traldi, Pietro; Bertani, Roberta; Facchin, Giacomo; Pandolfo, Luciano, Org.Mass Spectrom., CODEN: ORMSBG, 29(11), <1994>, 619-624; BABS-5944502

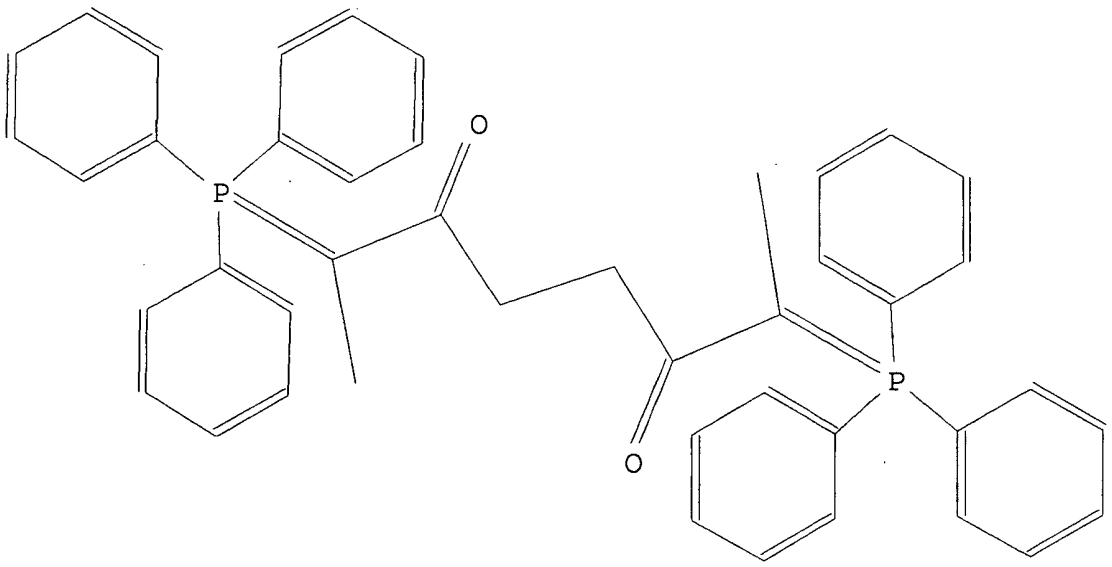
Reaction:
RX
Reaction ID (.ID): 3775143
Reactant BRN (.RBRN): 750218, 1697986
Reactant (.RCT): (triphenyl-.lambda.5-phosphanylidene)-acetonitrile, propadienedione
Product BRN (.PBRN): 6854445
Product (.PRO): 3,5-dioxo-2,6-bis-(triphenyl-.lambda.5-phosphanylidene)-heptanedinitrile
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 3775143.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 85 percent (BRN=6854445)
Solvent (.SOL): 1,2-dichloro-ethane
Other Conditions (.COND): Ambient temperature
Reference(s):
1. Pandolfo, Luciano; Facchin, Giacomo; Bertani, Roberta; Ganis, Paolo; Valle, Giovanni, Angew.Chem., CODEN: ANCEAD, 106(5), <1994>, 586-588; BABS-5894226

L16 ANSWER 9 OF 12 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN): 6459041
Chemical Name (CN): 2,7-bis-(triphenyl-.lambda.5-phosphanylidene)-octane-3,6-dione
Autonom Name (AUN): 2,7-bis-(triphenyl-.lambda.5-phosphanylidene)-octane-3,6-dione

Molec. Formula (MF):	C44 H40 O2 P2
Molecular Weight (MW):	662.75
Lawson Number (LN):	16731, 3764
Compound Type (CTYPE):	isocyclic
Constitution ID (CONSID):	5626219
Tautomer ID (TAUTID):	6164298
Beilstein Citation (BSO):	6-16
Entry Date (DED):	1994/01/24
Update Date (DUPD):	1994/01/24



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
IR	Infrared Spectrum	1
MP	Melting Point	1
NMR	Nuclear Magnetic Resonance	2

Reference(s):
1. Sanehi, Ram; Bansal, R. K.; Mehrotra, R. C., Indian J.Chem.Sect.A, CODEN: IJCADU, 24(5), <1985>, 398-402; BABS-5793414

Notes(s):
1. 1540 cm**(-1)

Reaction:
RX

Reaction ID (.ID):	3879158
Reactant BRN (.RBRN):	1773914, 958776
Reactant (.RCT):	1,4-dithio-succinic acid S,S'-diethyl ester, ethylidene-triphenyl-.lambda.5-phosphane
Product BRN (.PBRN):	6459041
Product (.PRO):	2,7-bis-(triphenyl-.lambda.5-phosphanylidene)-octane-3,6-dione
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	3879158.1
Reaction Classification (.CL):	Preparation
Yield (.YDT):	63 percent (BRN=6459041)
Solvent (.SOL):	toluene
Other Conditions (.COND):	1.) ambient temp., 5 h, 2.) reflux, 3 h

Reference(s):
1. Sanehi, Ram; Bansal, R. K.; Mehrotra, R. C., Indian J.Chem.Sect.A, CODEN: IJCADU, 24(5), <1985>, 398-402; BABS-5793414

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1	L1	279	harlan.xa.	USPAT
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4	L4	70	3 and binuclear	USPAT
5	L5	40	3 and ylide	USPAT
6	L6	0	3 and ylide and nickle	USPAT
7	L7	23	3 and ylide and nickel	USPAT
8	L8	2	3 and ylide and nickel and binuclear	USPAT
9	L9	1	("4691036").PN.	USPAT

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Dossier: 09936902

Legal Date: 11-26-2003

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1	CTFR	5

Total number of pages: 5

Remarks:

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